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Comment

Comment on the paper "Analysis of thermal expansivity of alkali halide crystals" : NaF as an example

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Singh and Chauhan [1] (SC) have questioned the validity of the Kumar formulation for the temperature dependence of thermal expansivity and claimed to report a new and better relation. It is found that neither the relation is new nor better. SC have copied the relation already reported in the literature, which was also used by Kushwah and Shanker [2]. The superiority of the relation claimed by SC is based on the imaginary experimental data created by them, which are not available in any reference cited by SC.

Recently, SC [1] acknowledged correctly that they having some valuable guidance from Shanker (refer to the acknowledgement of [1]), discovered a new relation for the temperature dependence of inter-atomic separation. SC also claimed that their formula gives the results which are in better agreement with the experimental data as compared with the relation reported by Kumar [3]. The relation reported by SC [1] reads as follows :

$$r = r_0 \exp\left[\frac{1}{3}\left\{\alpha_0 (T - T_0) + \frac{1}{2}\alpha' (T - T_0)^2\right\}\right] \quad (1)$$

which is based on the approximation

$$\alpha = \alpha_0 + \alpha' (T - T_0). \quad (2)$$

Here, the symbols have the same meaning as in Ref. [1]. The relation reported by Kumar [3] is the following :

$$r = r_0 \exp\left[\frac{1}{3}\left\{\alpha_0 (T - T_0) + \frac{1}{2}\alpha' \left(T^2 - T_0^2\right)\right\}\right] \quad (3)$$

which is based on the following simple approximation :

$$\alpha = \alpha_0 + \alpha' T \quad (4)$$

SC [1] claimed that they modified the formulation reported by Kumar (eq. 3) in the form of eq. (1), which is a new relation [1]. It is very interesting to quote the following statement from a paper of Shanker (refer to [2]) who guided them for such research. Using the notations of SC [1] this reads as follows [2].

"Guillermet and Gustafson [4] considered an exponential dependence of V/V_0 on temperature given below :

$$\frac{V}{V_0} = \exp\left[\left\{\alpha_0 (T - T_0) + \frac{1}{2}\alpha' (T - T_0)^2\right.\right. \quad (5)$$

which yields a linear dependence of α on temperature as follows :

$$\alpha = \alpha_0 + \alpha' (T - T_0), \quad (6)$$

where $V/V_0 = (r/r_0)^3$"

Kushwah and Shanker [2] used eq. (5) and reported the variation of V/V_0 *versus* T for MgO. Eq. (5) is exactly same as eq. (1). It seems that Shanker [2] did not remember his past contribution during his valuable guidance to SC [1] and encouraged them to call eq. (1)

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as a new one discovered by them. Thus, the statement of SC [1] that they investigated new relation (eq. 1) is misleading.

SC [1] stated that eq. (4) is not consistent with the boundary condition *viz.* $\alpha = \alpha_0$ at $T = T_0$. It seems that SC [1] is not aware about the 'boundary' condition, which correctly reads as $\alpha = \alpha_0$ at $T = 0$. Eq. (4) is truly consistent with the boundary condition. Thus, the statement of SC [1] regarding the boundary condition is not correct. SC [1] have calculated the values of interatomic separation r as a function of temperature T, to demonstrate that eq. (1) gives the better results as compared with eq. (3). This needs a critical analysis of their results [1]. For the purpose, we consider the case of NaF as an example. Using the input data as given by SC [1] and evaluating α' as $\alpha' = \alpha_0^2 \delta_T$, the results obtained from eqs. (1) and (3) are given in Table 1, which may be judged in the light of actual experimental data [5–7]. The imaginary experimental data of SC [1] are also given in Table 1.

Table 1. NaF : Calculated values of r (in Å) at different temperatures T (in K) using eqs. (1) and (3) along with the actual [7] and imaginary [1] experimental data. The percentage deviations (PD) calculated at highest temperature (900 K), are given in the last row, using actual experimental data [7].

T (K)	r (Å)		Experimental data	
	SC (eq. 1)	Kumar (eq. 3)	Actual [7]	Imaginary [1]
300	2.318	2.318	2.318	2.318
400	2.326	2.327	2.326	2.326
500	2.334	2.336	2.335	2.334
600	2.342	2.346	2.345	2.342
700	2.351	2.356	2.356	2.351
800	2.361	2.368	2.368	2.361
900	2.371	2.378	2.382	2.371
PD	0.50	0.16		

Note : The imaginary experimental data [1] means that these are not available in any reference quoted by SC [5–7], which are in cent per cent agreement with those calculated by SC (eq. 1).

It is found that the claim of SC [1] that eq. (1) is better than eq. (3) is flawed, but the reverse is true. To demonstrate this more clearly, we have also plotted the results in Figure 1. The percentage deviations at highest temperatures (900 K) are also reported in Table 1. It is found that to demonstrate the superiority of eq. (1), SC [1] have quoted the imaginary experimental data. These authors [1] have given three references in the support of experimental data *viz.* Enck *et al* [5], Enck and Dommel [6], He and Yan [7]. It is pertinent to mention here that Enck *et al* [5] studied only KCl, while Enck and Dommel

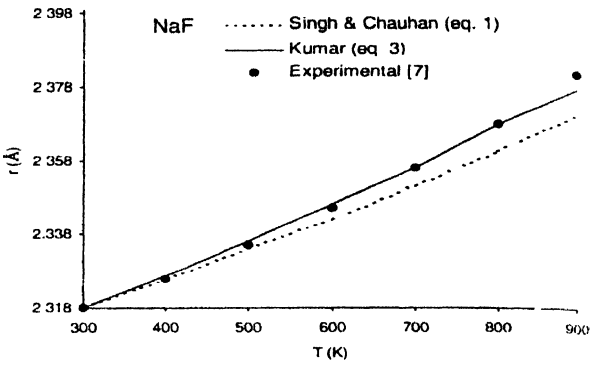

Figure 1. Temperature dependence of interatomic separation along with the actual experimental data [7].

[6] studied only NaCl, and the data used by SC [1] do not match with those given by He and Yan [7] (Table 1). Obviously, SC [1] have used the imaginary experimental data (not available in any reference) to mislead the readers, which are in cent percent agreement with the values calculated from eq. (1). Coming back to the work of Enck and Dommel [6] who determined the coefficient of linear thermal expansion α for NaCl and fitted their results to the polynomial of a particular form, which was further divided into two forms for low and high temperature regions [6]. This second order polynomial reads as follows (refer to eq. (5) of Enck and Dommel [6])

$$\alpha(T) = 3.912 \times 10^{-5} + 2.012 \times 10^{-8} T + 2.809 \times 10^{-11} T^2. \quad (7)$$

Writing eq. (7) in the mathematical form of symbols, we get

$$\alpha(T) = \alpha_0 + \alpha' T + \alpha'' T^2 . \quad (8)$$

Here, α_0, α' and α'' are constants as defined by eq. (7). The coefficient of linear thermal expansion is related to the interatomic distance by the following relation [3]

$$r = r_0 \exp \int_{T_0}^{T} \alpha(T)\, dT . \quad (9)$$

Combining eqs. (8) and (9), we get

$$r = r_0 \exp \left[\alpha_0 (T - T_0) + \frac{\alpha'}{2} \left(T^2 - T_0^2 \right) + \frac{\alpha''}{3} \left(T^3 - T_0^3 \right) \right]. \quad (10)$$

Here, it should be remembered that in eq. (10), α is the coefficient of linear thermal expansion whilst α is defined as the coefficient of volume thermal expansion in eqs.

(1, 3). Eq. (10) may be compared with the eqs. (1) and (3). By neglecting the higher order terms in eq. (10), we get exactly eq. (3), but not eq. (1). Thus, within the framework of the studies of Enck and Dommel [6] as referred by SC [1], eq. (1) is not justified while eq. (3) is justified.

On the basis of above studies, it may be concluded that the claim of SC [1] *viz.* they investigated eq. (1) which is better than eq. (3) is baseless and misleading because they have written the earlier published relation in their name and used the imaginary experimental data to show the superiority. Some other misleading statements have also been given by SC. For example, we may read the following lines [1] "Figures 2–4 : plots of $\Delta r = r(T) - r(T_o)$ in Å *versus* T in K for NaF, NaCl, KCl, KBr, KI, RbCl, RbBr and RbI crystals". It is shocking that the paper [1] contains only three plots *viz.* NaCl, KI and RbCl. Five plots of NaF, KCl, KBr, RbBr and RbI crystals are missing. This demonstrates the serious error in the statements given by these authors [1]. Not only this, the same paper [1] has been duplicated at same time somewhere else [8]. We shall like to submit a separate detailed analysis to the concerned Editor of Ref. [8].

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